EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	244	(556/404,560/262,568/11).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2007/10/01 08:47
L2	21	l1 and phosphonium	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2007/10/01 08:48

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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 02	LMEDLINE coverage updated
NEWS 3	JUL 02	SCISEARCH enhanced with complete author names
NEWS 4	JUL 02	CHEMCATS accession numbers revised
NEWS 5	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 6	JUL 16	CAplus enhanced with French and German abstracts
NEWS 7	JUL 18	CA/CAplus patent coverage enhanced
NEWS 8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9	JUL 30	USGENE now available on STN
NEWS 10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 11	AUG 06	BEILSTEIN updated with new compounds
NEWS 12	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 13	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 14	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 15	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 16	AUG 27	USPATOLD now available on STN
NEWS 17	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 18	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 19	SEP 13	FORIS renamed to SOFIS
NEWS 20	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 21	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 22	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 23	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:41:40 ON 01 OCT 2007

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
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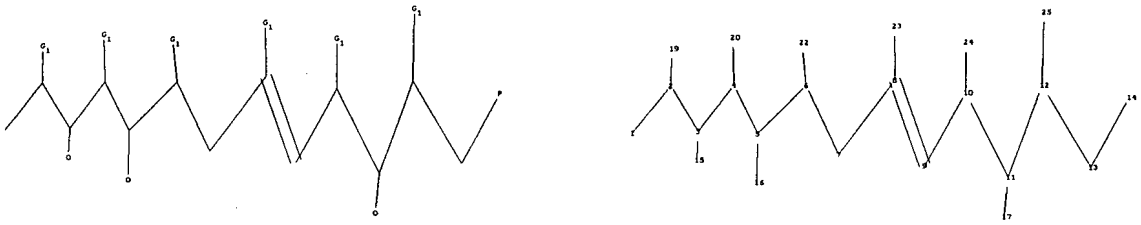

chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 19 20 22 23 24 25
chain bonds :
1-2 2-3 2-19 3-4 3-15 4-5 4-20 5-6 5-16 6-7 6-22 7-8 8-9 8-23 9-10
10-11 10-24 11-12 11-17 12-13 12-25 13-14
exact/norm bonds :
2-19 3-15 4-20 5-16 6-22 8-23 10-24 11-17 12-25
exact bonds :
1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14

G1:H,Ak

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
19:CLASS 20:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 08:42:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4 TO 200
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

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FULL SEARCH INITIATED 08:42:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L3 14 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
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FILE LAST UPDATED: 30 Sep 2007 (20070930/ED)

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=> s l3 full
L4 18 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1122416 CAPLUS
DOCUMENT NUMBER: 144:22752

TITLE: Design, Synthesis, and Biological Evaluation of Potent Discodermolide Fluorescent and Photoaffinity Molecular Probes

AUTHOR(S): Smith, Amos B., III; Rucker, Paul V.; Brouard, Ignacio; Freeze, B. Scott; Xia, Shujun; Horwitz, Susan Band

CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104, USA

SOURCE: Organic Letters (2005), 7(23), 5199-5202
CODEN: ORLEF7; ISSN: 1523-7060

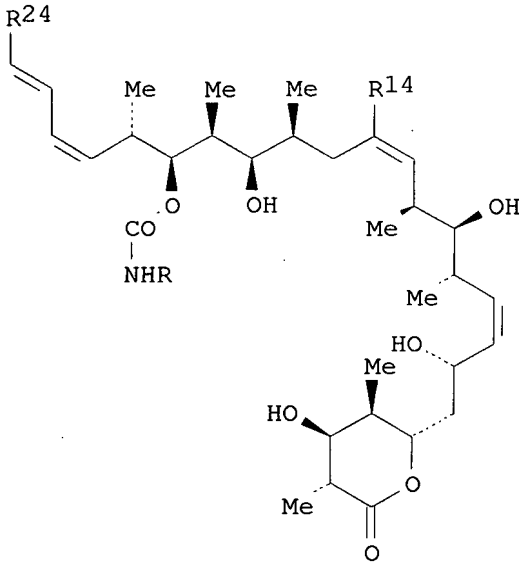
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:22752

GI



I

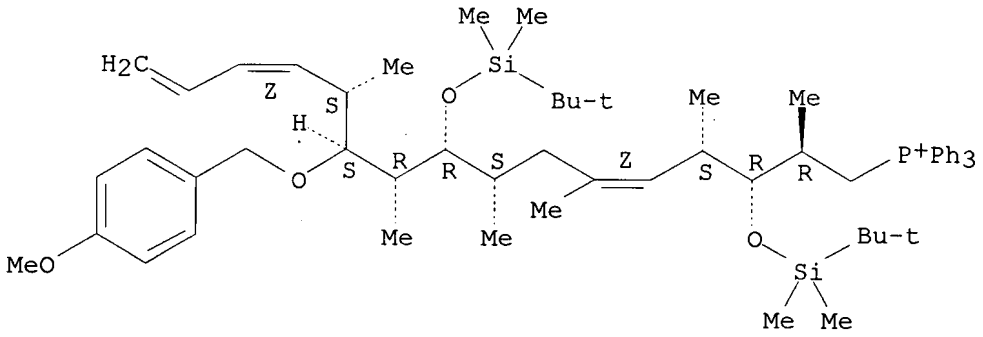
AB The design, synthesis, and biol. evaluation of a series of (+)-discodermolide mol. probes possessing photoaffinity and fluorescent appendages was achieved. Stereoselective olefin cross-metathesis comprised a key tactic for construction of two of the mol. probes. Three tritium labeled photoaffinity probes I (R = T-4-C6H4-CO-C6H4, R14 = Me, H, R24 = H; R = H, R14 = Me, R24 = T-4-C6H4-CO-4-C6H4CO2CH2) were prepared

IT 252342-54-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis, and biol. evaluation of potent discodermolide fluorescent and photoaffinity mol. probes)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

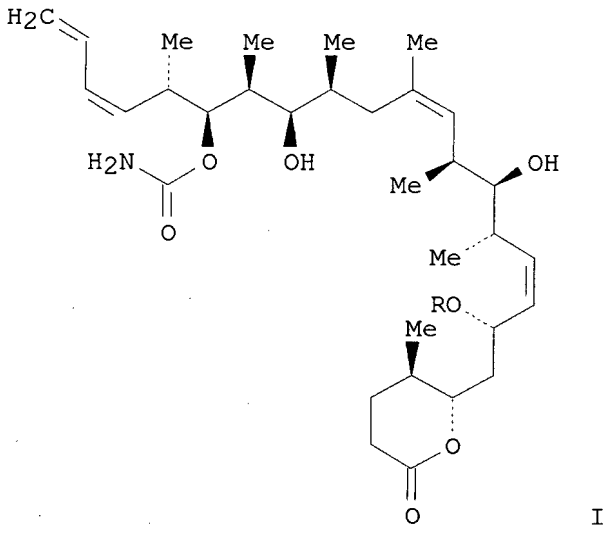
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



● I^-

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1080558 CAPLUS
DOCUMENT NUMBER: 144:6608
TITLE: Design, Synthesis, and Biological Evaluation of Simplified Analogues of (+)-Discodermolide. Additional Insights on the Importance of the Diene, the C(7) Hydroxyl, and the Lactone
AUTHOR(S): Smith, Amos B., III; Xian, Ming
CORPORATE SOURCE: Department of Chemistry, Monell Chemical Senses Center, and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Organic Letters (2005), 7(23), 5229-5232
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:6608
GI



I

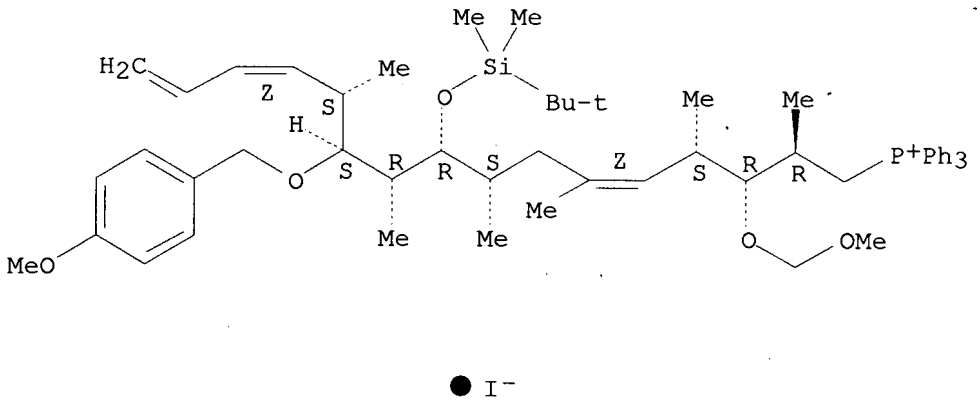
AB The design, synthesis, and biol. evaluation of seven totally synthetic analogs of the antitumor agent (+)-discodermolide are reported. For example, discodermolide analog I (R = H) reacted with methoxymethyl chloride to give I (R = CH2OMe) in 40% yield. Saturation of the terminal diene system, alteration of the substituents on the lactone, and alkylation of the C(7)-hydroxyl group reveal significant structure-activity relationships.

IT 633293-74-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (+)-discodermolide analogs, their antitumor activity, and structure-activity relationships)

RN 633293-74-0 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-(methoxymethoxy)-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

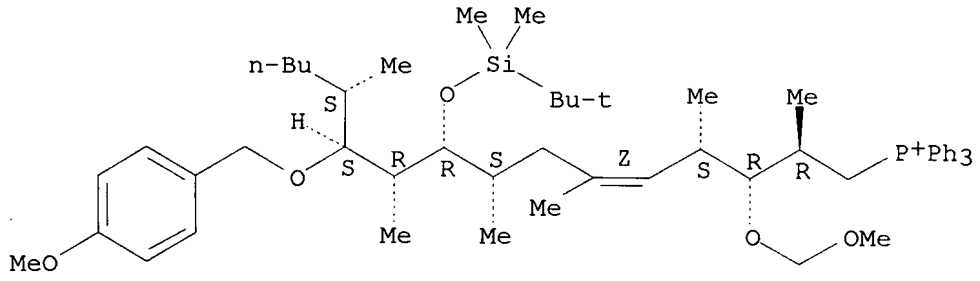
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 870074-99-0P 870075-28-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (+)-discodermolide analogs, their antitumor activity, and structure-activity relationships)

RN 870074-99-0 CAPLUS
CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-(methoxymethoxy)-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5-hexadecenyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

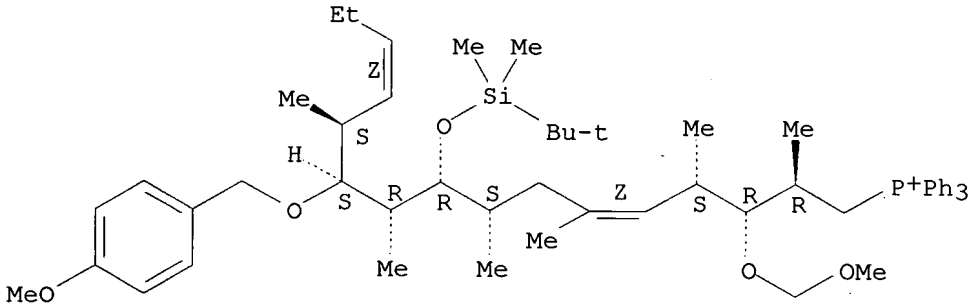
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



● I^-

RN 870075-28-8 CAPLUS
CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-(methoxymethoxy)-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13-hexadecadienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



● I^-

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:312870 CAPLUS
DOCUMENT NUMBER: 143:26411
TITLE: Toward Understanding How the Lactone Moiety of Discodermolide Affects Activity
AUTHOR(S): Shaw, Simon J.; Sundermann, Kurt F.; Burlingame, Mark A.; Myles, David C.; Freeze, B. Scott; Xian, Ming; Brouard, Ignacio; Smith, Amos B., III
CORPORATE SOURCE: Kosan Biosciences, Inc., Hayward, CA, 94545, USA

SOURCE: Journal of the American Chemical Society (2005), 127(18), 6532-6533
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:26411
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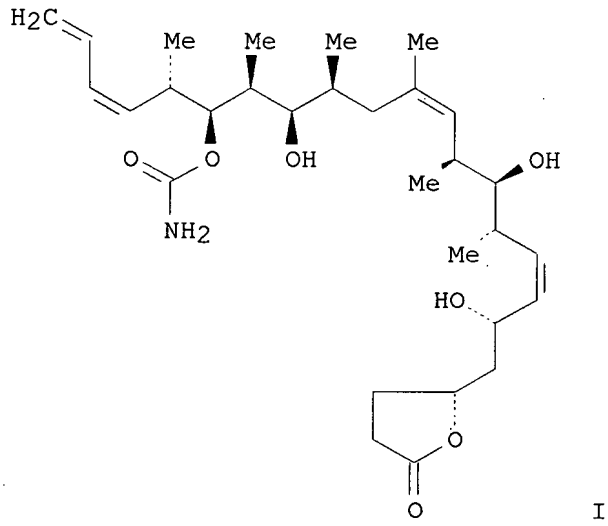


I

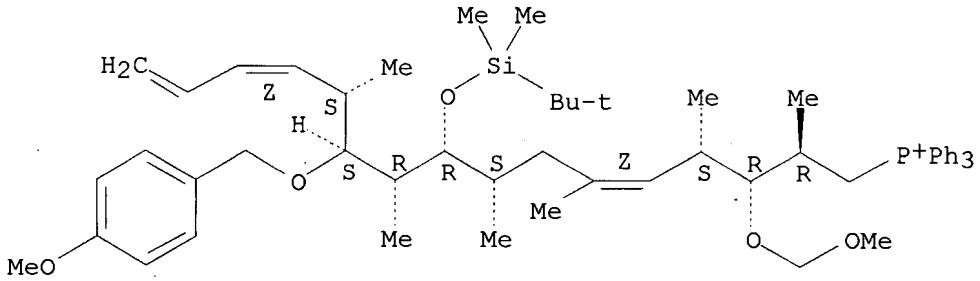
AB A series of simplified discodermolide analogs have been designed and synthesized in an attempt to understand the role of the lactone ring. These synthetic efforts have led to an unsubstituted butyrolactone I being generated, which shows improved activity over the natural product.

IT 633293-74-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and anticancer activity of discodermolide derivs.)

RN 633293-74-0 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-(methoxymethoxy)-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

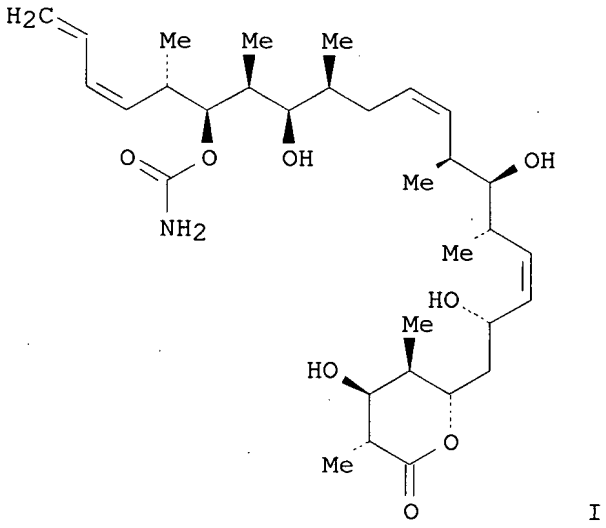
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



● I^-

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1141985 CAPLUS
DOCUMENT NUMBER: 142:197745
TITLE: Design, Synthesis, and Evaluation of Analogues of (+)-14-Normethyldiscodermolide
AUTHOR(S): Smith, Amos B., III; Freeze, B. Scott; LaMarche, Matthew J.; Hirose, Tomoyasu; Brouard, Ignacio; Xian, Ming; Sundermann, Kurt F.; Shaw, Simon J.; Burlingame, Mark A.; Horwitz, Susan Band; Myles, David C.
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Organic Letters (2005), 7(2), 315-318
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:197745
GI



I

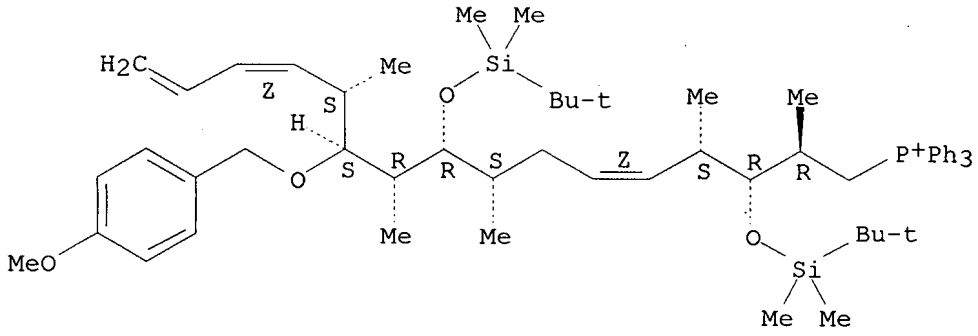
AB The design, syntheses, and biol. evaluation of nine totally synthetic analogs of the microtubule-stabilizing agent (+)-14-normethyldiscodermolide (I) are reported. Simplification at the C(21)-C(24) terminal diene and at the C(1)-C(5) lactone moieties reveals significant structure-activity relationships.

IT 835929-84-5P 837383-17-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design, synthesis, and biol. evaluation of analogs of (+)-14-normethyldiscodermolide)

RN 835929-84-5 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,8,10,12-pentamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

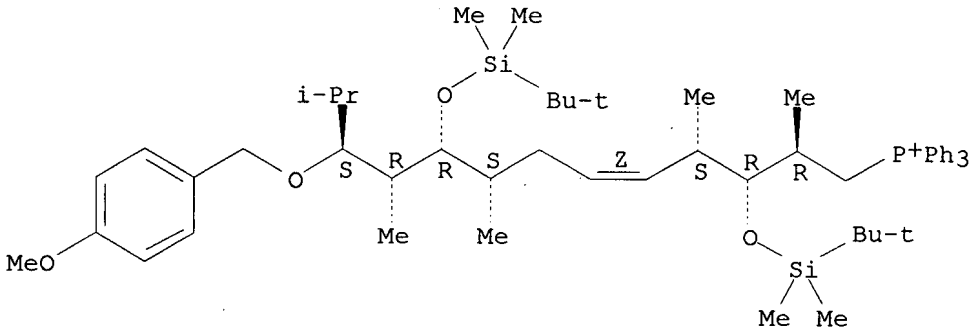


● I⁻

RN 837383-17-2 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,8,10,12-pentamethyl-5-tridecenyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



● I⁻

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1122299 CAPLUS
DOCUMENT NUMBER: 142:197742
TITLE: Design, Synthesis, and Evaluation of Carbamate-Substituted Analogues of (+)-Discodermolide
AUTHOR(S): Smith, Amos B., III; Freeze, B. Scott; LaMarche, Matthew J.; Hirose, Tomoyasu; Brouard, Ignacio; Rucker, Paul V.; Xian, Ming; Sundermann, Kurt F.; Shaw, Simon J.; Burlingame, Mark A.; Horwitz, Susan Band; Myles, David C.
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Organic Letters (2005), 7(2), 311-314
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:197742
GI

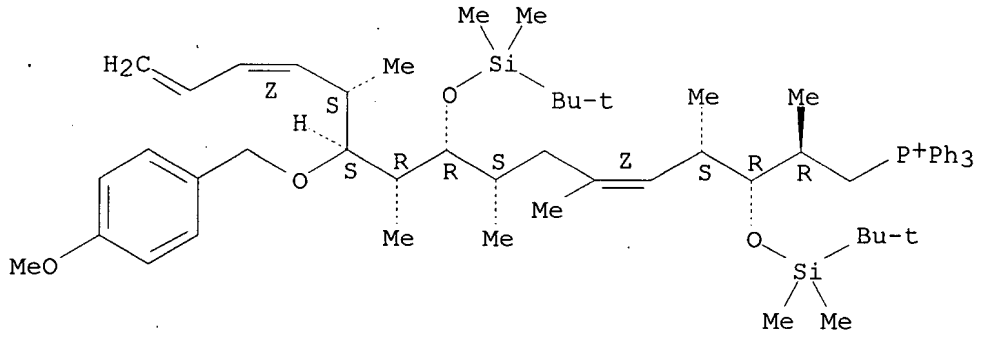
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The design, syntheses, and biol. evaluation of 22 totally synthetic analogs, e.g. I, of the potent microtubule-stabilizing agent (+)-discodermolide (II) have been achieved. Structure-activity relationships of the C(19)-carbamate were defined, exploiting two synthetically simplified scaffolds, as well as the parent (+)-discodermolide framework.

IT 252342-54-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(design, synthesis, and biol. evaluation of carbamate-substituted analogs of (+)-discodermolide)

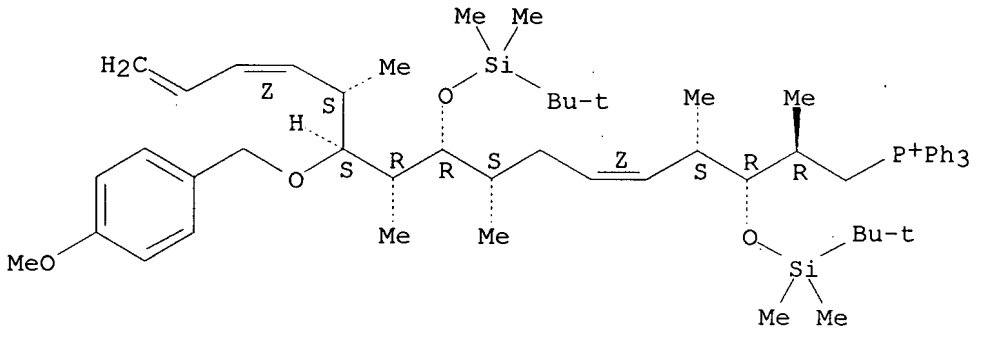
RN 252342-54-4 CAPLUS
CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 835929-84-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design, synthesis, and biol. evaluation of carbamate-substituted analogs of (+)-discodermolide)
RN 835929-84-5 CAPLUS
CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,8,10,12-pentamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1016004 CAPLUS
DOCUMENT NUMBER: 142:6360
TITLE: Synthetic techniques and intermediates for polyhydroxy dienyl lactones and mimics thereof
INVENTOR(S): Myles, David C.; Burlingame, Mark; Shaw, Simon James; Sundermann, Kurt F.; Freeze, Brian Scott; Martin, Ignacio Brouard; Hirose, Tomoyasu; Smith, Amos B.
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA

SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004101508	A2	20041125	WO 2004-US10272	20040402
WO 2004101508	A3	20050303		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005049414	A1	20050303	US 2004-817532	20040402
PRIORITY APPLN. INFO.:			US 2003-460744P P	20030402
			US 2003-476378P P	20030606

OTHER SOURCE(S): CASREACT 142:6360; MARPAT 142:6360
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

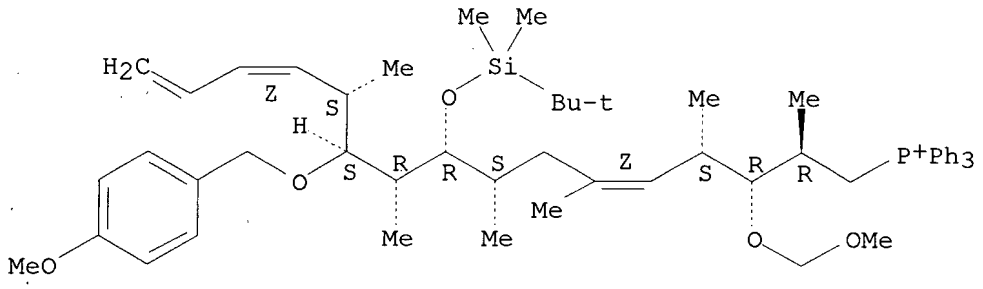
AB Synthetic methods and intermediates, e.g., I·X- [R0 = C1-6-alkyl, C2-6-alkenyl, C2-6-alkynyl, (CH2)r(C3-6-cycloalkyl), CH2-aryl, CH2-heterocycle; r = 0 - 4; R1, R2, R3, R6, R7, R8 = H, C1-10-alkyl; R4 = acid-labile OH protecting group; R5 = oxidatively-labile OH protecting group; R9 = C6-14-aryl; Q = H, acid-labile OH protecting group; (whereby the acid-labile OH protecting group has a mass of 135 Daltons or less and is unbranched at the atom bonded to O of the protected OH); X = halogen], useful in the preparation of lactone containing compds. such as discodermolide and compds. which mimic the chemical or biol. activity of discodermolide are provided. The synthetic method comprises reaction of halide II with phosphine P(R9)3 for a time and under conditions sufficient to prepare I·X- (whereby the pressure is less than about 10,000 psi). Thus, I·X- [R0 = CH:CHCH:CH2-(Z), R1 = R2 = R3 = R6 = R7 = R8 = Me, R4 = CH2C6H4OMe-4, R5 = Q = SiMe2CMe3, R9 = Ph, X = I] was prepared and used to synthesize (+)-discodermolide (III) via Wittig reaction with aldehyde IV.

IT 633293-74-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of, with (oxotetrahydropyranyl)propanal derivative; synthetic techniques and intermediates for discodermolide and other polyhydroxy dienyl lactones and mimics thereof)

RN 633293-74-0 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-(methoxymethoxy)-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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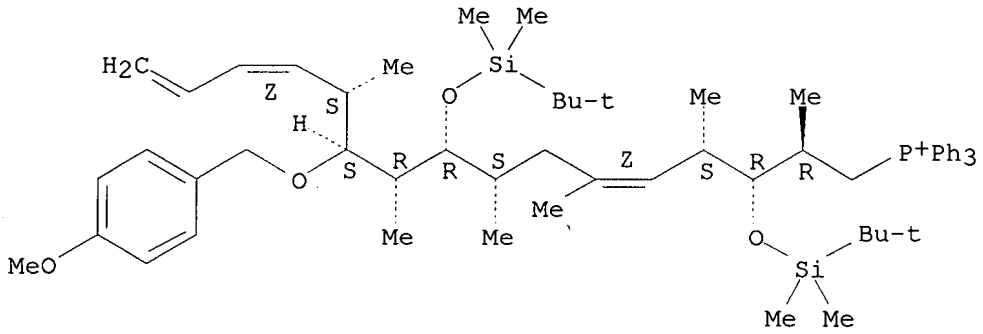
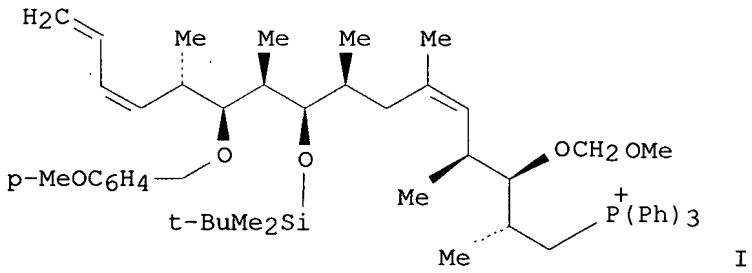
L4 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:303318 CAPLUS
DOCUMENT NUMBER: 141:54112
TITLE: Design, synthesis and cytotoxicity of 7-deoxy aryl discodermolide analogues
AUTHOR(S): Burlingame, Mark A.; Shaw, Simon J.; Sundermann, Kurt F.; Zhang, Dan; Petryka, Joseph; Mendoza, Esteban; Liu, Fenghua; Myles, David C.; LaMarche, Matthew J.; Hirose, Tomoyasu; Freeze, B. Scott; Smith, Amos B.
CORPORATE SOURCE: Department of Chemistry, Kosan Biosciences Inc., Hayward, CA, 94545, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2335-2338
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:54112
AB A series of 7-deoxy discodermolide analogs in which the lactone fragment C' was replaced by aryl substituents were designed, synthesized, and evaluated for cytotoxicity.
IT 252342-54-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(design, synthesis and antitumor cytotoxicity of 7-deoxy aryl discodermolide analogs)
RN 252342-54-4 CAPLUS
CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:810303 CAPLUS
DOCUMENT NUMBER: 140:27700
TITLE: A Practical Improvement, Enhancing the Large-Scale Synthesis of (+)-Discodermolide: A Third-Generation Approach
AUTHOR(S): Smith, Amos B.; Freeze, B. Scott; Brouard, Ignacio; Hirose, Tomoyasu
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Organic Letters (2003), 5(23), 4405-4408
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:27700
GI



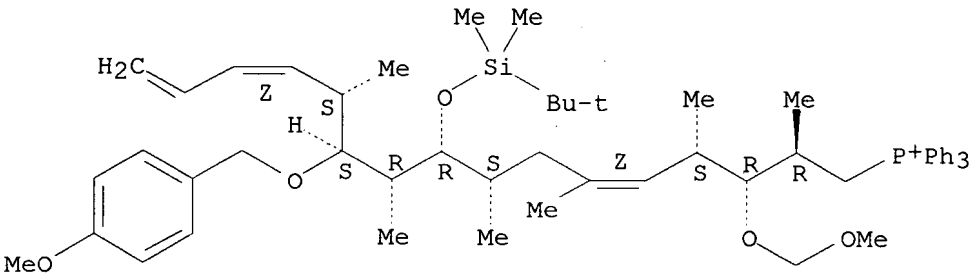
I

AB A significant improvement to the Penn one-gram synthesis of (+)-discodermolide has been achieved. Specifically, reduction of the steric bulk of the C(11) hydroxyl protecting group permits formation of the requisite AB Wittig salt I at the expense of the undesired intramol. cyclization upon treatment with PPh3 at ambient pressure.

IT 633293-74-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(large-scale synthesis of (+)-discodermolide, a third-generation approach)

RN 633293-74-0 CAPLUS
CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-(methoxymethoxy)-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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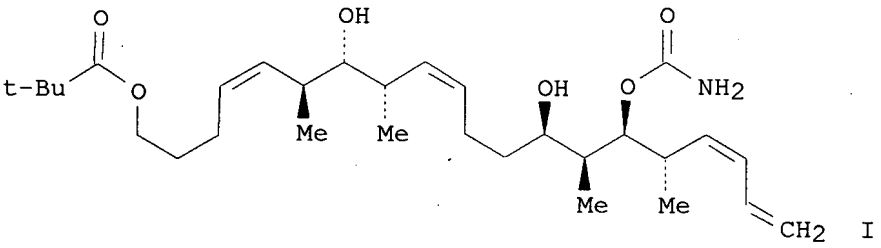
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:500684 CAPLUS
DOCUMENT NUMBER: 139:381288
TITLE: Synthesis and biological assessment of simplified analogues of the potent microtubule stabilizer (+)-Discodermolide
AUTHOR(S): Minguez, Jose M.; Kim, Sun-Young; Giuliano, Kenneth A.; Balachandran, Raghavan; Madiraju, Charitha; Day, Billy W.; Curran, Dennis P.
CORPORATE SOURCE: Department of Chemistry, Chevron Science Center, Pittsburgh, PA, 15260, USA
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(15), 3335-3357
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:381288
GI



I

AB An efficient, convergent and stereocontrolled synthesis of simplified analogs (e.g. I) of the potent antimitotic agent (+)-discodermolide has

been achieved and several small libraries have been prepared In all the libraries, the discodermolide Me groups at C14 and C16 and the C7 hydroxy group were removed and the lactone was replaced by simple esters. Other modifications introduced in each series of analogs were related to C11, C17 and C19 of the natural product. Key elements of the synthetic strategy included (a) elaboration of the main subunits from a common intermediate and (b) fragment couplings using Wittig reactions to install the (Z)-olefins. Library components were analyzed for microtubule-stabilizing actions in vitro, for displacement of [3H]paclitaxel from its binding site on tubulin, for antiproliferative activity against human carcinoma cells, and for cell signaling and mitotic spindle alterations by a multiparameter fluorescence cell-based screening technique. The results show that even significant structural simplification can lead to analogs with actions related to microtubule targeting.

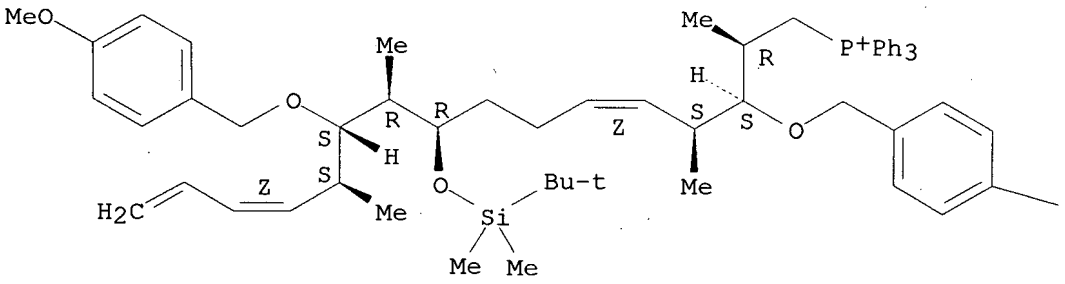
IT 623926-76-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. activity of discodermolide analogs)

RN 623926-76-1 CAPLUS

CN Phosphonium, [(2R,3S,4S,5Z,9R,10R,11S,12S,13Z)-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,11-bis[(4-methoxyphenyl)methoxy]-2,4,10,12-tetramethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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PAGE 1-B

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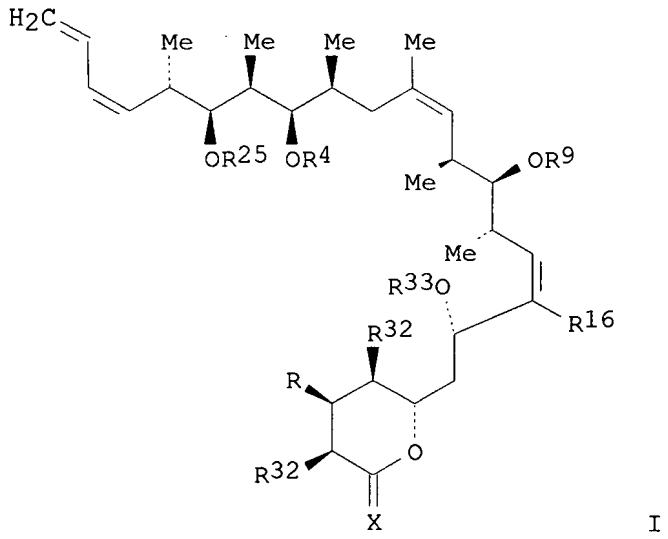
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:133020 CAPLUS
DOCUMENT NUMBER: 138:170004
TITLE: Preparation of compounds which mimic the chemical and biological properties of discodermolide
INVENTOR(S): Smith, Amos B., III; Beauchamp, Thomas J.; Lamarche, Matthew J.; Rucker, Paul
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA
SOURCE: PCT Int. Appl., 333 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003013502	A1	20030220	WO 2002-US24932	20020806
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2456553	A1	20030220	CA 2002-2456553	20020806
AU 2002323029	A1	20030224	AU 2002-323029	20020806
EP 1414434	A1	20040506	EP 2002-756985	20020806
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1541096	A	20041027	CN 2002-815661	20020806
JP 2005526689	T	20050908	JP 2003-518511	20020806
US 2004048894	A1	20040311	US 2003-296138	20030602
ZA 2004000974	A	20050505	ZA 2004-974	20040205
IN 2004KN00289	A	20060331	IN 2004-KN289	20040304
PRIORITY APPLN. INFO.:			US 2001-310555P P	20010807
			WO 2002-US24932 W	20020806

OTHER SOURCE(S): MARPAT 138:170004
GI



I

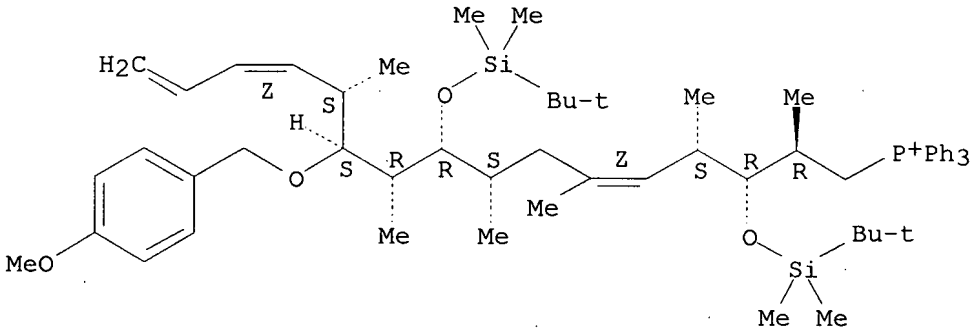
AB Discodermolide analogs, such as I [R = H, OR33; X = H2, O; R4, R9, R33 = H, acid labile protecting group; R25 = H, carbamoyl, thiocarbamoyl, oxidatively labile protecting group; R16, R32 = H, alkyl], were prepared Synthetic routes to both (-)- and (+)-discodermolide were presented. The prepared discodermolide analogs were assayed in vitro for tubulin polymerization inhibition and for cytotoxicity against human A459 cancer cells.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of compds. which mimic the chemical and biol. properties of discodermolide for pharmaceutical use as anticancer agents)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:575783 CAPLUS
DOCUMENT NUMBER: 137:125048
TITLE: Preparation of compounds which mimic the chemical and biological properties of discodermolide
INVENTOR(S): Smith, Amos B., III; Beauchamp, Thomas J.; Lamarche, Matthew J.
PATENT ASSIGNEE(S): The Trustees of The University of Pennsylvania, USA
SOURCE: U.S. Pat. Appl. Publ., 127 pp., Cont.-in-part of U. S. Ser. No. 455,649.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002103387	A1	20020801	US 2000-730929	20001206
US 6870058	B2	20050322		
US 5789605	A	19980804	US 1996-759817	19961203
US 6031133	A	20000229	US 1998-21878	19980211
US 6242616	B1	20010605	US 1999-455649	19991207
CA 2431045	A1	20020613	CA 2001-2431045	20011206
WO 2002046150	A2	20020613	WO 2001-US47958	20011206
WO 2002046150	A3	20060105		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 200227375	A	20020618	AU 2002-27375	20011206
EP 1585725	A2	20051019	EP 2001-996231	20011206
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AU 2002300472	A1	20030213	AU 2002-300472	20020730
ZA 2003004259	A	20050425	ZA 2003-4259	20030530
IN 2003KN00715	A	20051202	IN 2003-KN715	20030604
US 2005065353	A1	20050324	US 2004-779049	20040213
WO 2005079378	A2	20050901	WO 2005-US4643	20050211
WO 2005079378	A3	20060216		
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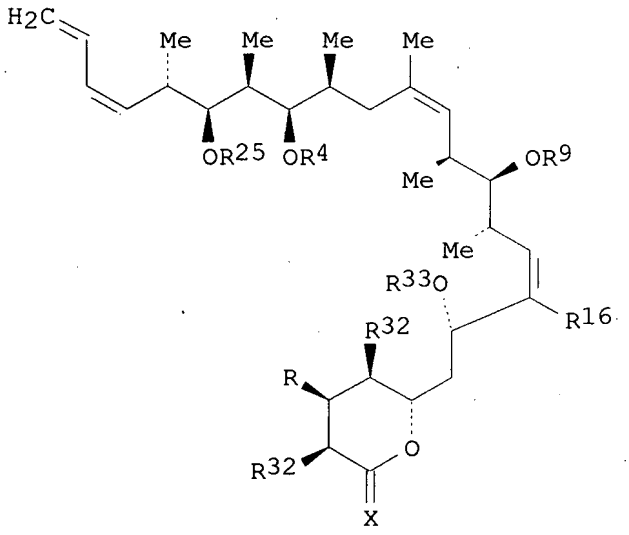
US 2007043223	A1	20070222	US 2006-486344	20060713

PRIORITY APPLN. INFO.:

US 1996-759817	A2 19961203
US 1998-21878	A2 19980211
US 1999-455649	A2 19991207
US 1998-121551	A2 19980723

AU 1999-52190 A3 19990720
US 2000-730929 A 20001206
WO 2001-US47958 W 20011206
US 2004-779049 A 20040213

OTHER SOURCE(S): MARPAT 137:125048
GI



I

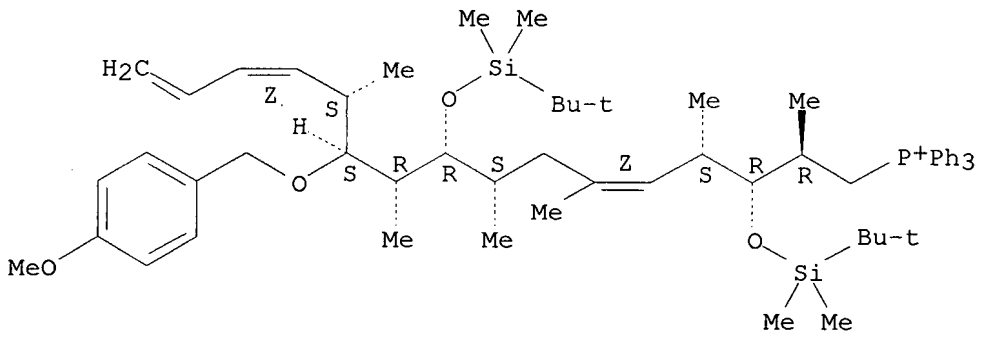
AB Discodermolide analogs, such as I [R = H, OR33; X = H2, O; R4, R9, R33 = H, acid labile protecting group; R25 = H, oxidatively labile protecting group; R16, R32 = H, alkyl], were prepared Synthetic routes to both (-)- and (+)-discodermolide were presented.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of compds. which mimic the chemical and biol. properties of discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:449643 CAPLUS
DOCUMENT NUMBER: 137:33164
TITLE: Preparation of compounds which mimic the chemical and biological properties of discodermolide
INVENTOR(S): Smith, Amos B., III; Beauchamp, Thomas J.; Lamarche, Matthew J.
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania Center for Technology Transfer, USA
SOURCE: PCT Int. Appl., 267 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002046150	A2	20020613	WO 2001-US47958	20011206
WO 2002046150	A3	20060105		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2002103387	A1	20020801	US 2000-730929	20001206
US 6870058	B2	20050322		
CA 2431045	A1	20020613	CA 2001-2431045	20011206
AU 200227375	A	20020618	AU 2002-27375	20011206
EP 1585725	A2	20051019	EP 2001-996231	20011206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
AU 2002300472	A1	20030213	AU 2002-300472	20020730
IN 2003KN00715	A	20051202	IN 2003-KN715	20030604
WO 2005079378	A2	20050901	WO 2005-US4643	20050211
WO 2005079378	A3	20060216		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM

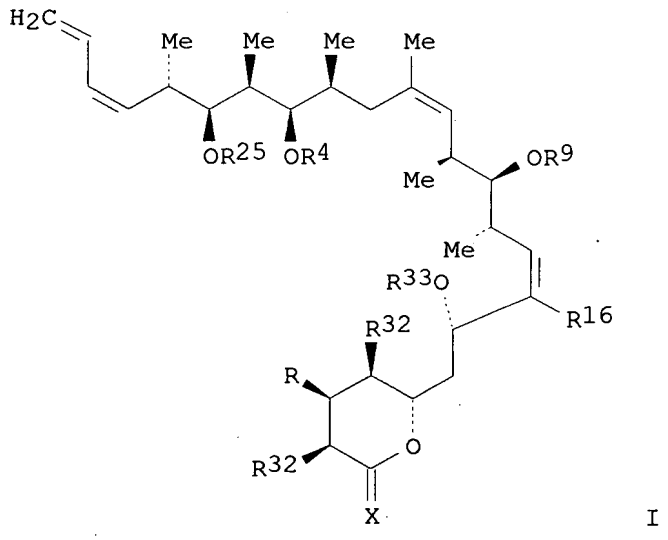
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2000-730929	A 20001206
US 1996-759817	A2 19961203
US 1998-21878	A2 19980211
AU 1999-52190	A3 19990720
US 1999-455649	A2 19991207
WO 2001-US47958	W 20011206
US 2004-779049	A 20040213

OTHER SOURCE(S): MARPAT 137:33164

GI



I

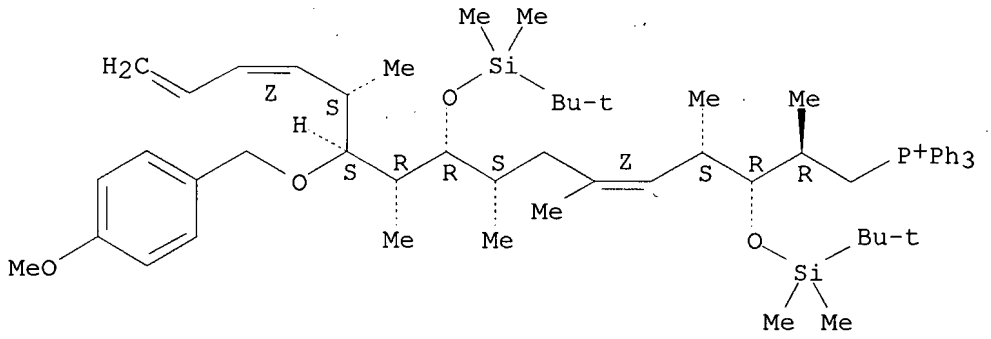
AB Discodermolide analogs, such as I [R = H, OR33; X = H2, O; R4, R9, R33 = H, acid labile protecting group; R25 = H, oxidatively labile protecting group; R16, R32 = H, alkyl], were prepared Synthetic routes to both (-)- and (+)-discodermolide were presented.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of compds. which mimic the chemical and biol. properties of discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

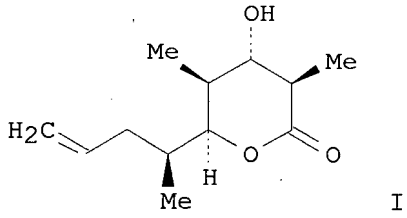


● I^-

L4 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:123244 CAPLUS
DOCUMENT NUMBER: 136:183657
TITLE: Process for the biomediated preparation of intermediates for use in the synthesis of polyketides, such as epothilone D and discodermolide
INVENTOR(S): Santi, Daniel V.; Ashley, Gary; Myles, David C.
PATENT ASSIGNEE(S): Kosan Biosciences, Inc., USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012534	A2	20020214	WO 2001-US25112	20010809
WO 2002012534	A3	20020906		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO 2001092991	A2	20011206	WO 2001-US17352	20010529
WO 2001092991	A3	20020808		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001075012	A5	20011211	AU 2001-75012	20010529
CA 2417358	A1	20020214	CA 2001-2417358	20010809
AU 2001083275	A5	20020218	AU 2001-83275	20010809

EP 1307579 A2 20030507 EP 2001-962062 20010809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004520008 T 20040708 JP 2002-517818 20010809
PRIORITY APPLN. INFO.: US 2000-224038P P 20000809
US 2000-237382P P 20001004
US 2000-248387P P 20001113
US 2001-867845 A 20010529
US 2000-207331P P 20000530
WO 2001-US17352 W 20010529
WO 2001-US25112 W 20010809
OTHER SOURCE(S): CASREACT 136:183657; MARPAT 136:183657
GI



I

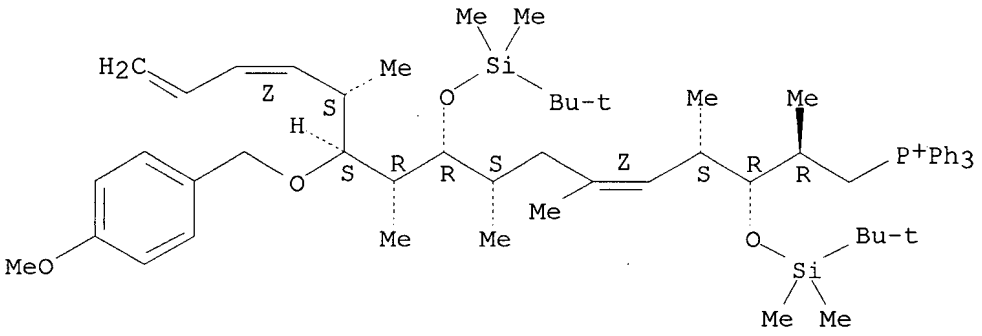
AB The present invention relates to compds., such as I, made by a subset of modules from one or more polyketide synthase ("PKS") genes that are used as starting material in the chemical synthesis of novel mols., particularly naturally occurring polyketides or derivs. thereof. The biol. derived intermediates ("bio-intermediates") generally represent particularly difficult compds. to synthesize using traditional chemical approaches due to one or more stereocenters. In one aspect of the invention, an intermediate in the synthesis of epothilone is provided that feeds into the synthetic protocol of Danishefsky and co-workers. In another aspect of the invention, intermediates in the synthesis of discodermolide are provided that feed into the synthetic protocol of Smith and co-workers. By taking advantage of the inherent stereochem. specificity of biol. processes, the syntheses of key intermediates and thus the overall syntheses of compds. like epothilone and discodermolide are greatly simplified.

IT 252342-54-4P
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(process for the biomediated preparation of intermediates for use in the synthesis of polyketides, such as epothilone D and discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



● I^-

L4 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:412212 CAPLUS
DOCUMENT NUMBER: 135:19496
TITLE: Preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivatives for pharmaceutical use
INVENTOR(S): Smith, Amos B., III; Beauchamp, Thomas J.; Lamarche, Matthew J.; Arimoto, Hirokazu
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA
SOURCE: U.S., 126 pp., 6096904 Cont.-in-part of U.S. 6,096,904.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6242616	B1	20010605	US 1999-455649	19991207
US 5789605	A	19980804	US 1996-759817	19961203
US 6031133	A	20000229	US 1998-21878	19980211
US 6096904	A	20000801	US 1998-121551	19980723
CA 2393968	A1	20010614	CA 2000-2393968	20001206
WO 2001042179	A1	20010614	WO 2000-US32996	20001206
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002103387	A1	20020801	US 2000-730929	20001206
US 6870058	B2	20050322		
EP 1248761	A1	20021016	EP 2000-983924	20001206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003531110	T	20031021	JP 2001-543482	20001206
AU 2002300472	A1	20030213	AU 2002-300472	20020730
US 2005065353	A1	20050324	US 2004-779049	20040213
WO 2005079378	A2	20050901	WO 2005-US4643	20050211

WO 2005079378 A3 20060216
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2007043223 A1 20070222 US 2006-486344 20060713
PRIORITY APPLN. INFO.: US 1996-759817 A1 19961203
US 1998-21878 A1 19980211
US 1998-121551 A2 19980723
AU 1999-52190 A3 19990720
US 1999-455649 A 19991207
US 2000-730929 A1 20001206
WO 2000-US32996 W 20001206
US 2004-779049 A 20040213
OTHER SOURCE(S): CASREACT 135:19496; MARPAT 135:19496
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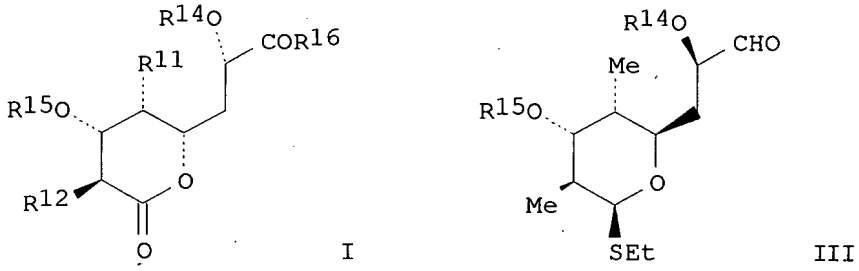
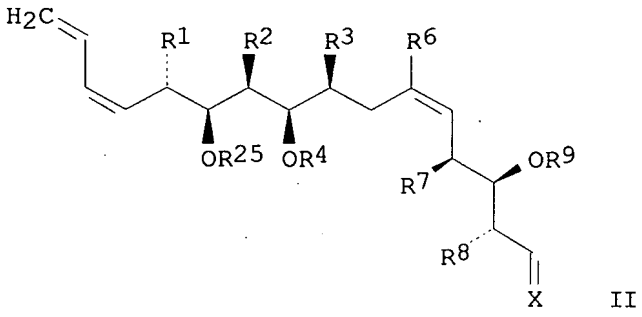




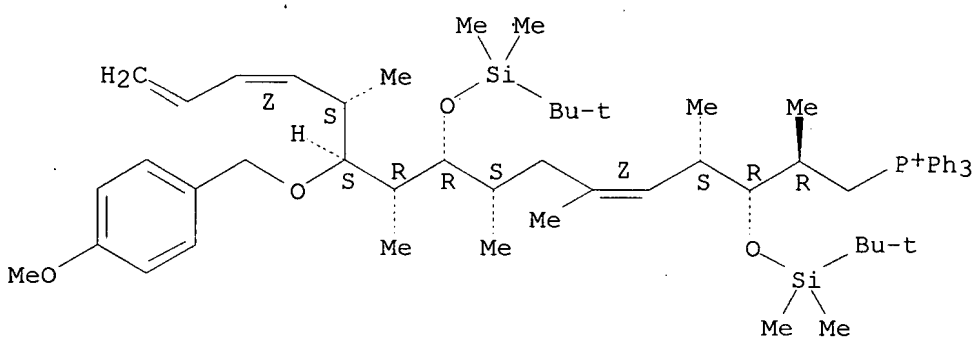
AB Preparation of intermediates, such as I [R11, R12 = alkyl; R14, R15 = acid labile protecting groups; R16 = H, alkyl] and II [R1, R2, R7, R8 = alkyl; R3, R6, R16 = H, alkyl; R4, R9 = acid labile hydroxyl protecting group; R25 = oxidatively labile hydroxyl protecting group; X = :C(J)R16, a Wittig olefination formed from a pyranylalkyl ketone, such as I and II (X = P+Ph3I-)], for the synthesis of discodermolides and their analogs, which are useful as pharmaceuticals, was presented. Thus, synthon III (R14 = R15 = SiMe2CMe3) was prepared via a multistep synthetic sequence starting from (2R)-3-hydroxy-2-methylpropanoic acid Me ester. The synthetic utility of II was subsequently demonstrated by its use in the preparation of (-)-discodermolide.
IT 252342-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivs. for pharmaceutical use)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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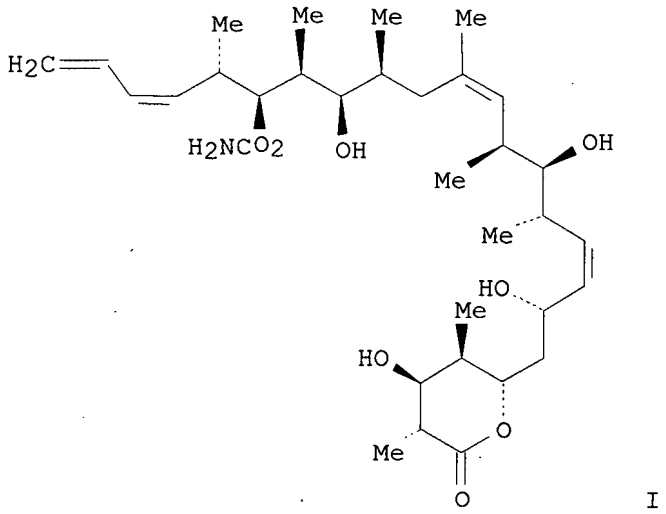
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:597937 CAPLUS
DOCUMENT NUMBER: 133:335118
TITLE: Evolution of a Gram-Scale Synthesis of (+)-Discodermolide
AUTHOR(S): Smith, Amos B., III; Beauchamp, Thomas J.; LaMarche, Matthew J.; Kaufman, Michael D.; Qiu, Yuping; Arimoto, Hirokazu; Jones, David R.; Kobayashi, Kaoru
CORPORATE SOURCE: Department of Chemistry Monell Chemical Senses Center and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Journal of the American Chemical Society (2000), 122(36), 8654-8664
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:335118
GI



I

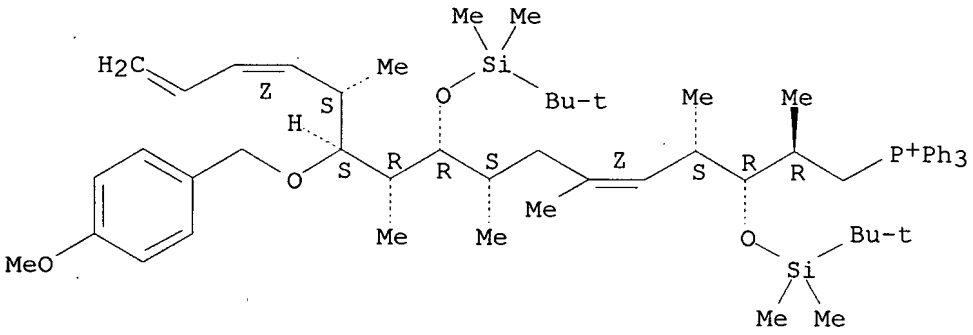
AB An efficient, highly convergent, stereocontrolled total synthesis of the potent antimitotic agent (+)-discodermolide (I) has been achieved on gram scale. Key elements of the successful strategy include (1) elaboration of three advanced fragments from a common precursor (CP) which embodies the repeating stereochem. triad of the discodermolide backbone, (2) σ-bond installation of the Z trisubstituted olefin, exploiting a modified Negishi cross-coupling reaction, (3) synthesis of a late-stage phosphonium salt utilizing high pressure, and (4) Wittig installation of the Z disubstituted olefin and the terminal (Z)-diene.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(evolution of a gram-scale synthesis of (+)-discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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REFERENCE COUNT: 101 THERE ARE 101 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:531688 CAPLUS
DOCUMENT NUMBER: 133:135166
TITLE: Preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivatives for pharmaceutical use
INVENTOR(S): Smith, Amos B., III; Qiu, Yuping; Kaufman, Michael; Arimoto, Hirokazu; Jones, David R.; Kobayashi, Kaoru; Beauchamp, Thomas J.
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA
SOURCE: U.S., 83 pp., Cont.-in-part of U.S. 5,789,605.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6096904	A	20000801	US 1998-121551	19980723
US 5789605	A	19980804	US 1996-759817	19961203
CA 2338310	A1	20000203	CA 1999-2338310	19990720
WO 2000004865	A2	20000203	WO 1999-US16369	19990720
WO 2000004865	A3	20000921		
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AU 9952190	A	20000214	AU 1999-52190	19990720
AU 749844	B2	20020704		
EP 1105383	A2	20010613	EP 1999-937330	19990720
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JP 2002521317	T	20020716	JP 2000-560858	19990720
US 6242616	B1	20010605	US 1999-455649	19991207
AU 2002300472	A1	20030213	AU 2002-300472	20020730
US 2005065353	A1	20050324	US 2004-779049	20040213
WO 2005079378	A2	20050901	WO 2005-US4643	20050211
WO 2005079378	A3	20060216		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
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US 2007043223	A1	20070222	US 2006-486344	20060713
AU 2006203417	A1	20060831	AU 2006-203417	20060808

PRIORITY APPLN. INFO.:

US 1996-759817	A2	19961203
US 1998-21878	A1	19980211
US 1998-121551	A	19980723
AU 1999-52190	A3	19990720
WO 1999-US16369	W	19990720
US 1999-455649	A2	19991207
US 2000-730929	A1	20001206
AU 2002-300472	A	20020730
US 2004-779049	A	20040213

OTHER SOURCE(S): MARPAT 133:135166
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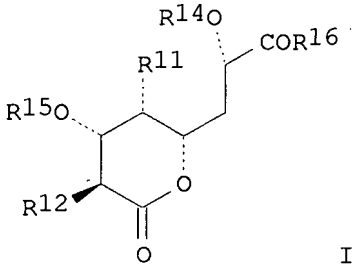

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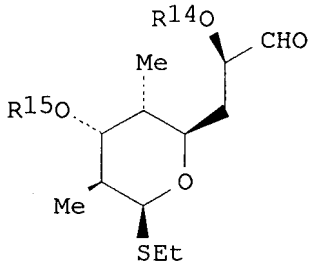


II

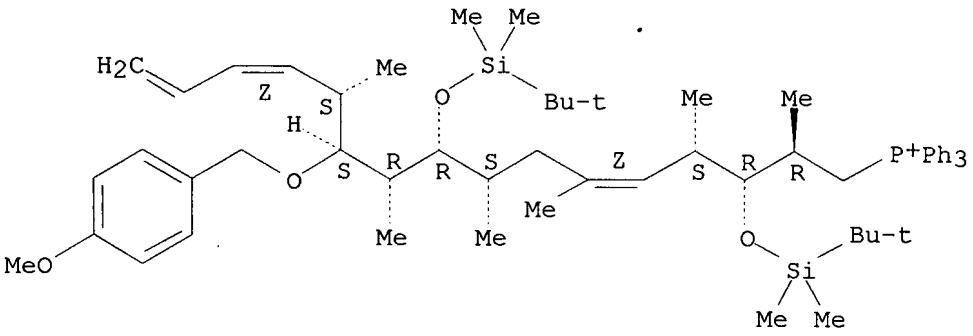
AB Preparation of intermediates, such as I [R11, R12 = alkyl; R14, R15 = acid labile protecting groups; R16 = H, alkyl], for the synthesis of discodermolides and their analogs, which are useful as pharmaceuticals, was presented. Thus, synthon II (R14 = R15 = SiMe2CMe3) was prepared via a multistep synthetic sequence starting from (2R)-3-hydroxy-2-methylpropanoic acid Me ester. The synthetic utility of II was subsequently demonstrated by its use in the preparation of (-)-discodermolide.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivs. for pharmaceutical use)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:84572 CAPLUS
DOCUMENT NUMBER: 132:137207
TITLE: Preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone

derivatives for pharmaceutical use

INVENTOR(S): Smith, Amos B., III; Qiu, Yuping; Kaufman, Michael; Arimoto, Hirokazu; Jones, David R.; Kobayashi, Kaoru; Beauchamp, Thomas J.

PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA

SOURCE: PCT Int. Appl., 201 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

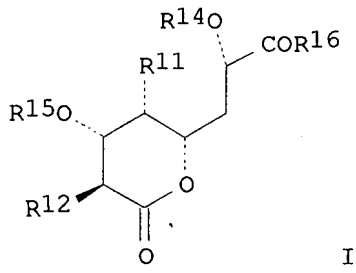
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000004865	A2	20000203	WO 1999-US16369	19990720
WO 2000004865	A3	20000921		
W: AU, CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6096904	A	20000801	US 1998-121551	19980723
CA 2338310	A1	20000203	CA 1999-2338310	19990720
AU 9952190	A	20000214	AU 1999-52190	19990720
AU 749844	B2	20020704		
EP 1105383	A2	20010613	EP 1999-937330	19990720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002521317	T	20020716	JP 2000-560858	19990720
AU 2002300472	A1	20030213	AU 2002-300472	20020730
WO 2005079378	A2	20050901	WO 2005-US4643	20050211
WO 2005079378	A3	20060216		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:		
US 1998-121551	A	19980723
US 1996-759817	A2	19961203
AU 1999-52190	A3	19990720
WO 1999-US16369	W	19990720
US 2004-779049	A	20040213

OTHER SOURCE(S): MARPAT 132:137207

GI



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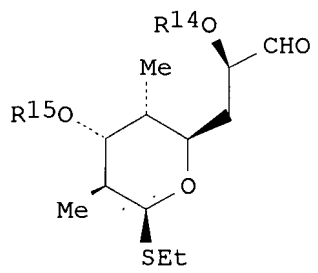


II

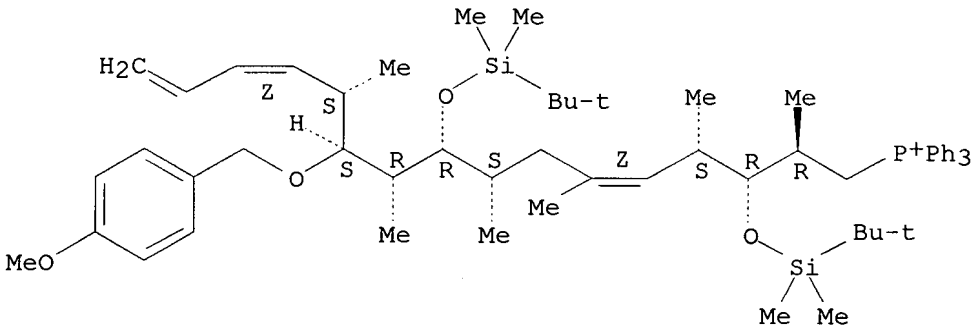
AB Preparation of intermediates, such as I [R11, R12 = alkyl; R14, R15 = acid labile protecting groups; R16 = H, alkyl], for the synthesis of discodermolides and their analogs, which are useful as pharmaceuticals, was presented. Thus, synthon II (R14 = R15 = SiMe2CMe3) was prepared via a multistep synthetic sequence starting from (2R)-3-hydroxy-2-methylpropanoic acid Me ester. The synthetic utility of II was subsequently demonstrated by its use in the preparation of (-)-discodermolide.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivs. for pharmaceutical use)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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L4 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:694867 CAPLUS
DOCUMENT NUMBER: 132:35548
TITLE: Gram-Scale Synthesis of (+)-Discodermolide
AUTHOR(S): Smith, Amos B., III; Kaufman, Michael D.; Beauchamp, Thomas J.; LaMarche, Matthew J.; Arimoto, Hirokazu
CORPORATE SOURCE: Department of Chemistry Monell Chemical Senses Center and Laboratory for Research on the Structure of Matter, University of Pennsylvania, PA, 19104, USA
SOURCE: Organic Letters (1999), 1(11), 1823-1826
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

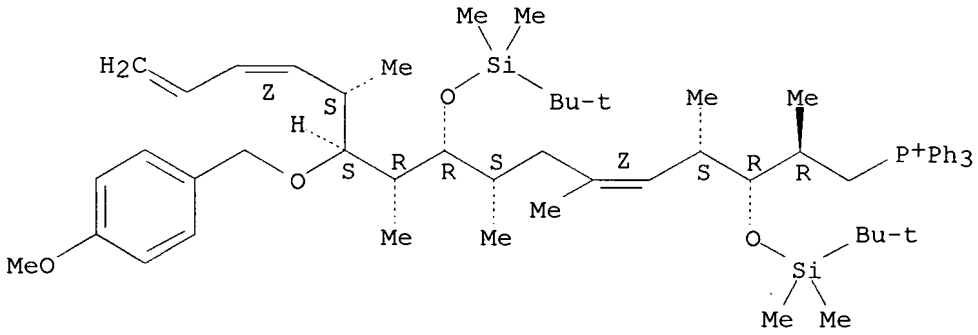
AB A triply convergent, highly efficient second-generation synthesis of the potent antimitotic agent (+)-discodermolide has been achieved on a 1-g scale.

IT 252342-54-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(gram-scale synthesis of (+)-discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



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REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 08:41:40 ON 01 OCT 2007)

FILE 'REGISTRY' ENTERED AT 08:41:47 ON 01 OCT 2007
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 14 S L1 FULL

FILE 'CAPLUS' ENTERED AT 08:42:18 ON 01 OCT 2007
L4 18 S L3 FULL

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